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A neural network representation of the potential energy surface in Si- and Si-Li systems BRAD MALONE, EKIN CUBUK, School of Engineering and Applied Sciences, Harvard University, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — A recently developed technique for extending calculations to longer length and time scales is based upon the training of the biologically-inspired neural network machine learning architecture to reproduce the potential energy surface. Trained with ab-initio density functional theory information, such neural networks can reproduce DFT-level accuracy in the study of processes traditionally limited to empirical potentials. We describe progress in constructing accurate neural network potentials for both elemental Si systems as well as Si systems which incorporate Li, the latter being of great current interest because of the promise of Si as an anode material in Li-ion batteries. These potentials allow for the study of interesting phase transformation behavior that occurs in these systems inaccessible by traditional approaches.

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